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SEMIGROUP ASYMPTOTICS, FUNK-HECKE IDENTITY AND THE GEGENBAUER COEFFICIENTS ASSOCIATED WITH THE SPHERICAL LAPLACIAN

STUART DAY AND ALI TAHERI

ABSTRACT. A trace formulation of the Maclaurin spectral coefficients of the Schwartzian kernel of functions of the spherical Laplacian is given. A class of polynomials $\mathscr{P}_l^\nu(X)$ ($l \ge 0, \nu > -1/2$) linking to the classical Gegenbauer polynomials through a differential-spectral identity is introduced and its connection to the above spectral coefficients and their asymptotics analysed. The paper discusses some applications of these ideas combined with the Funk-Hecke identity and semigroup techniques to geometric and variational-energy inequalities on the sphere and presents some examples.

1. Introduction. Let $(\mathscr{X}, g)$ be a smooth compact n-dimensional Riemannian manifold without boundary and let $\Delta = \Delta_g$ denote the Laplace-Beltrami operator on $\mathscr{X}$ given in local coordinates via

$$\Delta_g = (\det g)^{-1} \sum \partial_j \left(\sum \sqrt{\det g}\, g^{jk} \partial_k \right). \tag{1.1}$$

By basic spectral theory there is a complete orthonormal basis $(\varphi_k : k \ge 0)$ of eigenfunctions of $-\Delta_g$ in $L^2(\mathscr{X}, dv_g)$ with associated eigenvalues $(\lambda_k : k \ge 0)$ verifying $-\Delta_g \varphi_k = \lambda_k \varphi_k$. Each λ_k has finite multiplicity and the spectrum $\Sigma(-\Delta_g)$ can be arranged in ascending order $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots$ with $\lambda_j \nearrow \infty$. Furthermore by orthogonality $(\varphi_j, \varphi_k)_{L^2(\mathscr{X})} = 0$ for $0 \le j \ne k$ whilst $||\varphi_j||_{L^2(\mathscr{X})} = 1$ for all $j \ge 0$.

Now for a given function $\Phi = \Phi(X)$ in the Borel functional calculus of $-\Delta_g$ the Schwartzian (or integral) kernel of the operator $\Phi(-\Delta_g)$ can be expressed by the spectral sum $\sum \Phi(\lambda_k)\, \varphi_k \otimes \varphi_k$, or more specifically,

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the sum

$$K_\Phi(x,y) = \sum_{k=0}^{\infty} \Phi(\lambda_k)\varphi_k(x)\varphi_k(y), \qquad x,y \in \mathscr{X}. \tag{1.2}$$

In case of the heat semigroup $\Phi(X) = e^{-tX}$ $(t > 0)$ the analysis of the heat kernel and its asymptotics has been the subject of numerous investigations that has led to deep and profound results whose applications range from fields as diverse as direct and inverse spectral theory, index theory, number theory and automorphic forms to quantum field theory and many more. Indeed to comment further the short time asymptotics of the heat kernel of a compact Riemannian manifold was first studied in detail by Minakshisundaram and Pleijel in **[23]** through the construction of the so-called heat parametrix which then resulted in the formulation of the spectral zeta function $\zeta_{\mathscr{X}} = \zeta_{\mathscr{X}}(s)$ on $\mathscr{X}$ and a complete description of its poles and residues. As the heat semigroup is of trace class it has a well-defined and finite-valued trace whose short time asymptotics ($t \searrow 0$) takes the form **[23]** (*cf.* also **[7, 13]**)

$$\begin{aligned} \operatorname{tr} T(t) = \operatorname{tr} e^{t\Delta_g} &= \int_M K(t,x,x)\, dv_g(x) \\ &= \sum_{k=0}^{\infty} e^{-\lambda_k t} \sim \sum_{k=0}^{\infty} \frac{a_k^n(\mathscr{X}) t^k}{(4\pi t)^{n/2}}. \end{aligned} \tag{1.3}$$

The sequence of scalars $(a_k^n : k \geq 0)$ called the heat coefficients or the heat invariants (also known as the Minakshisundaram-Pleijel heat coefficients) associated with $(\mathscr{X}, g)$ are geometric invariants that can be entirely described through the Riemann curvature tensor R and its successive covariant derivatives. For instance the leading coefficient a_0^n is always the volume $\mathrm{Vol}_g(\mathscr{X})$, a_1^n is a constant multiple of the total scalar curvature (see below) and the further terms become increasingly more complicated integrals of polynomial expressions in R and its derivatives (see, e.g., **[7, 12, 13]**, **[19, 20]** for further detail on heat coefficients and local heat invariants and for some deep and far reaching implications see **[10, 11]**, **[16, 27, 30, 31]**). In particular and as a consequence the first few terms in the heat trace expansion (1.3) can be written as ($t \searrow 0$)

$$\Theta(t) = \operatorname{tr} T(t) = \sum_{k=0}^{\infty} e^{-\lambda_k t} \sim \frac{1}{(4\pi t)^{n/2}} \left\{ \mathrm{Vol}_g(\mathscr{X}) + t \int_M \frac{\mathrm{Scal}}{6}\, dv_g \right.$$

$$\left. + t^2 \int_M \frac{5\mathrm{Scal}^2 + 2|\mathrm{Ric}|^2 + 2|\mathrm{R}|^2 + \Delta_g \mathrm{Scal}}{360}\, dv_g + O\left(t^3\right) \right\} \tag{1.4}$$

where R, Ric and Scal denote the Riemann curvature tensor, the Ricci curvature and the scalar curvature of $(\mathscr{X}, g)$ and $|\mathrm{R}|$, $|\mathrm{Ric}|$ are the norms of R, Ric respectively. (See **[20]**, **[22]**.)

In case of a compact rank one symmetric space $\mathscr{X} = G/K$ of a compact Lie group G and with K the isotropy group of a point in $\mathscr{X}$, starting from the spectral sum (1.2) and using the addition formula for the matrix coefficients of irreducible unitary representations it can be seen that the Schwartzian kernel $K_\Phi(x, y)$ takes the form

$$K_\Phi(\theta) = \frac{1}{\mathrm{Vol}(\mathscr{X})} \sum_{k=0}^{\infty} M_k^n \Phi_k(\theta; \mathscr{X}) \Phi(\lambda_k^n), \tag{1.5}$$

where $\Phi_k = \Phi_k(\theta; \mathscr{X})$ are the spherical functions on $\mathscr{X}$, $\lambda_k^n = \lambda_k^n(\mathscr{X})$ are the numerically *distinct* eigenvalues of the Laplacian on $\mathscr{X}$, $M_k^n = M_k^n(\mathscr{X})$ is the dimension of the eigenspace associated with λ_k^n, $\theta = \theta(x, y)$ is the distance between the points $x, y \in \mathscr{X}$ and $\mathrm{Vol}(\mathscr{X})$ denotes the volume of $\mathscr{X}$. Specialising further to the n-sphere $\mathscr{X} = \mathbb{S}^n$ (note the identification $\mathbb{S}^n = \mathbf{SO}(n+1)/\mathbf{SO}(n)$) it is seen that the spherical or zonal functions here can be expressed via the *normalised* Gegenbauer polynomials (*see* Appendix A) as $\Phi_k = \mathscr{C}_k^\nu(\cos\theta)$ (with $\nu = (n-1)/2$) where as eigenfunctions $-\Delta \Phi_k = \lambda_k^n \Phi_k$ while $\Phi_k(0) = 1$ [*cf.* (A.4), (A.6)]. Hence (1.5) leads to

$$K_\Phi(\theta) = \frac{1}{\omega_n} \sum_{k=0}^{\infty} (2k+n-1) \frac{(k+n-2)!}{k!(n-1)!} \Phi(k(k+n-1)) \mathscr{C}_k^{\frac{n-1}{2}}(\cos\theta) \tag{1.6}$$

where $\lambda_k^n = k(k+n-1)$ with $k \geq 0$ are the distinct eigenvalues of $-\Delta$ on $\mathbb{S}^n$, $M_k^n = (2k+n-1)(k+n-2)!/(k!(n-1)!)$ is the multiplicity of λ_k^n, $\cos\theta = x \cdot y$ and $\omega_n = vol(\mathbb{S}^n) = 2\pi^{(n+1)/2}/\Gamma((n+1)/2)$. Now in view of the Schwartzian kernel K_Φ being an even function, subject to sufficient regularity, it admits a formal Maclaurin expansion about

$\theta = 0$ as

$$\sum_{l=0}^{\infty} \frac{\partial^{2l}}{\partial \theta^{2l}} K_\Phi \bigg|_{\theta=0} \frac{\theta^{2l}}{(2l)!} = \frac{1}{\omega_n} \sum_{l=0}^{\infty} \frac{b_{2l}^n}{(2l)!} \theta^{2l}. \tag{1.7}$$

The Maclaurin spectral coefficients $b_{2l}^n = b_{2l}^n[\Phi]$ can be described explicitly by invoking a spectral-differential identity proved in Theorem 2.1 below. Indeed it follows as a result that $b_0^n = \operatorname{tr} \Phi(-\Delta)$ while for $l \geq 1$ and with $\nu = (n-1)/2$,

$$b_{2l}^n = \frac{\partial^{2l}}{\partial \theta^{2l}} K_\Phi \bigg|_{\theta=0} = \sum_{k=0}^{\infty} M_k^n \Phi(\lambda_k^n) \sum_{j=1}^{l} \mathsf{c}_j^l [\lambda_k^n]^j = \operatorname{tr} [\Phi \mathscr{P}_l](-\Delta), \tag{1.8}$$

where $\mathscr{P}_l = \mathscr{P}_l^\nu(X)$ (with $l \geq 1$) is the degree l polynomial in X given explicitly by (2.3). The above identity and its variants along with further representations, including via Jacobi theta series, are further explored in Section 3. In Section 4 we study the asymptotics of the Maclaurin spectral coefficients through those of the heat invariants and theta series that in particular enables us to recover some associated heat asymptotics. In Section 5 as a further application we study semigroups generated by functions of the spherical Laplacian and a new class of geometric inequalities resulting from them. Here with the aid of the Funk-Hecke identity we are able to obtain further insight into the nature of the associated Maclaurin spectral coefficients and the structure of the variational inequalities.

2. The differential action $\mathsf{P}(d/d\theta)\mathscr{C}_k^\nu(\cos\theta)$ and the associated polynomials $\mathscr{P}_l^\nu = \mathscr{P}_l^\nu(X)$. Let $\mathsf{P} = \mathsf{P}_d(X)$ be a polynomial of degree $d \geq 2$ with a choice of coefficients $\mathsf{A}_0, \dots, \mathsf{A}_d$; specifically, $\mathsf{P}(X) = \sum \mathsf{A}_i X^i$, with $0 \leq i \leq d$, and the associated constant coefficient differential operator $\mathscr{L}$, defined formally by,

$$\mathscr{L} = \mathsf{P}(d/d\theta) = \sum_{i=0}^{d} \mathsf{A}_i d^i/d\theta^i. \tag{2.1}$$

In the following the differential operator $\mathscr{L}$ will be applied to the Gegenbauer polynomial which then results in an interesting differential-spectral identity that motivates the introduction of a new scale of polynomials.

Theorem 2.1. *For $\mathscr{L} = \mathsf{P}(d/d\theta)$ as in (2.1), the normalised Gegenbauer polynomial $\mathscr{C}_k^\nu$ with $k \geq 1$, $\nu > -1/2$ satisfies the identity,*

$$\mathsf{P}(d/d\theta)\mathscr{C}_k^\nu(\cos\theta)\Big|_{\theta=0} = \mathsf{A}_0 + \sum_{l=1}^{[d/2]} \mathsf{A}_{2l} \sum_{j=1}^{l} \mathsf{c}_j^l(\nu)[\lambda_k^\nu]^j$$

$$= \mathsf{A}_0 + \sum_{l=1}^{[d/2]} \mathsf{A}_{2l} \mathscr{P}_l^\nu(\lambda_k^\nu), \tag{2.2}$$

where $\lambda_k^\nu = k(k+2\nu)$ are the eigenvalues of the Gegenbauer operator (A.4). Furthermore the polynomial $\mathscr{P}_l^\nu = \mathscr{P}_l^\nu(X)$ and its scalar coefficients $\mathsf{c}_j^m(\nu)$ are given by

$$\mathscr{P}_l^\nu(X) = \sum_{j=1}^{l} \mathsf{c}_j^l(\nu) X^j, \qquad \mathsf{c}_j^l(\nu) = \sum_{m=j}^{l} \frac{2^m\Gamma(\nu+m)\Gamma(2\nu)\mathsf{b}_j^m}{\Gamma(\nu)\Gamma(2\nu+2m)} \mathsf{B}_{2l,m}(\zeta), \tag{2.3}$$

where b_j^m are defined recursively as: $\mathsf{b}_m^m = 1$, $\mathsf{b}_0^m = 0$ for $m \geq 1$ and $\mathsf{b}_j^{m+1} = \mathsf{b}_{j-1}^m - m(m+2\nu)\mathsf{b}_j^m$ for $1 \leq j \leq m$ and $\zeta = (\zeta_k)$ is the sequence $\zeta_k = (-1)^{k/2}$ for k even and zero otherwise.

Proof. Since $\mathscr{C}_k^\nu(\cos\theta)$ is an even function all its odd derivatives vanish at $\theta = 0$ and so we are left with the even derivatives. Using Faà de Bruno's formula (B.3) and (B.1) we have $[d^{2l}C_k^\nu(\cos\theta)/d\theta^{2l}]|_{\theta=0} = \sum_{m=1}^{l}[d^m C_k^\nu(t)/dt^m]|_{t=1}\mathsf{B}_{2l,m}(\zeta)$ for $l \geq 1$. Next using the recursive relation (A.3) (with $m \geq 1$) we have for ζ as expressed in the statement of the proposition

$$\frac{d^{2l}}{d\theta^{2l}} C_k^\nu(\cos\theta)\Big|_{\theta=0} = \sum_{m=1}^{l} \frac{\Gamma(\nu+m)}{2^{-m}\Gamma(\nu)} C_{k-m}^{\nu+m}(1)\mathsf{B}_{2l,m}(\zeta)$$

$$= \sum_{m=1}^{l} \mathsf{a}_m^l \frac{\Gamma(2\nu+k+m)k!}{\Gamma(2\nu+k)(k-m)!} C_k^\nu(1), \tag{2.4}$$

where we have used $C_k^\nu(1) = \Gamma(k+2\nu)/[\Gamma(2\nu)k!]$ and set

$$\mathsf{a}_m^l = \frac{2^m\Gamma(\nu+m)\Gamma(2\nu)}{\Gamma(\nu)\Gamma(2\nu+2m)} \mathsf{B}_{2l,m}(\zeta). \tag{2.5}$$

Now it is a straightforward matter to show, using induction, that the recursively defined scalars b_j^m satisfy

$$\prod_{p=0}^{m-1}(X - p(p+2\nu)) = \sum_{j=1}^{m} \mathsf{b}_j^m X^j. \tag{2.6}$$

As a result we can write the multiplicity functions as

$$\frac{\Gamma(2\nu+k+m)k!}{\Gamma(2\nu+k)(k-m)!} = \prod_{p=0}^{m-1}(k+2\nu+p)\prod_{p=0}^{m-1}(k-p) = \sum_{j=1}^{m} \mathsf{b}_j^m [k(k+2\nu)]^j. \tag{2.7}$$

Therefore by combining (2.4) and (2.7) we arrive at the differential-spectral identity

$$\frac{d^{2l}}{d\theta^{2l}} \mathscr{C}_k^\nu(\cos\theta)\bigg|_{\theta=0} = \sum_{m=1}^{l} \mathsf{a}_m^l \sum_{j=1}^{m} \mathsf{b}_j^m [k(k+2\nu)]^j = \mathscr{P}_l^\nu(\lambda_k^\nu). \tag{2.8}$$

Applying the differential operator $\mathsf{P}(d/d\theta)$ by taking into account only its even order terms combined with the above gives at once gives the desired conclusion. □

A straightforward set of calculations give the first few polynomials $\mathscr{P}_l^\nu$ that for the convenience of the reader are listed below. Indeed for $1 \le l \le 3$ we have

$$\mathscr{P}_1^\nu(X) = \frac{-X}{(2\,\nu+1)}, \qquad \mathscr{P}_2^\nu(X) = \frac{3X^2 - 4\nu X}{4\,\nu^2 + 8\,\nu + 3}, \tag{2.9}$$

$$\mathscr{P}_3^\nu(X) = \frac{-15X^3 + 60\nu X^2 - 16(4\nu^2+\nu)X}{8\,\nu^3 + 36\,\nu^2 + 46\,\nu + 15}, \tag{2.10}$$

while for $\mathscr{P}_4^\nu(X)$ is given by

$$\frac{105X^4 - 840\nu X^3 + 336\left(7\nu^2+2\nu\right)X^2 - 64\left(34\nu^3+24\nu^2+5\nu\right)X}{16\nu^4 + 128\nu^3 + 344\nu^2 + 352\nu + 105}. \tag{2.11}$$

3. A trace formulation of Maclaurin coefficients. Being motivated to understand and describe the Macluarin spectral coefficients more explicitly and in particular to formulate and exploit their relationship to the well-known heat trace and the Minakshisundaram-Plejel heat coefficients we now specialise to functions $\Phi = \Phi(X)$ of the Laplace transform type

$$\Phi(X) = \int_0^\infty e^{-Xs} f(s)\, ds, \qquad X \geq 0, \tag{3.1}$$

for a suitable L^1-integrable function f. For Φ as above using Fubini's Theorem to commute the integral and the summation we can write the Maclaurin spectral coefficients b_{2l}^n in (1.8) as

$$\begin{aligned} b_{2l}^n[\Phi] &= \int_0^\infty \sum_{k=0}^\infty M_k^n \sum_{j=1}^l \mathsf{c}_j^l [\lambda_k^n]^j e^{-\lambda_k^n s} f(s)\, ds \\ &= \int_0^\infty \sum_{j=1}^l \mathsf{c}_j^l (-1)^j f(s) \frac{d^j}{ds^j} \operatorname{tr} e^{s\Delta}\, ds \\ &= \int_0^\infty f(s) \left[\mathscr{P}_l^\nu \left(-\frac{d}{ds} \right) \right] \operatorname{tr} e^{s\Delta}\, ds. \end{aligned} \tag{3.2}$$

As a result one can now write the Macluarin spectral coefficients in the alternative and more suggestive trace form

$$b_{2l}^n = \operatorname{tr} [F_l^\nu(-\Delta)] \tag{3.3}$$

where F_l^ν is the function

$$F_l^\nu(X) := \int_0^\infty f(s) \mathscr{P}_l^\nu \left(-\frac{d}{ds} \right) e^{-sX}\, ds, \qquad X \geq 0. \tag{3.4}$$

Theorem 3.1. *Let $n \geq 2$ and let $\Phi = \Phi(X)$ be as defined by the Laplace integral* (3.1) *for a suitable integrable f. Consider the Schwartzian kernel of $\Phi(-\Delta)$ and its expansion*

$$K_\Phi(\theta) = \frac{1}{\omega_n} \sum_{k=0}^\infty M_k^n \Phi(\lambda_k^n) \mathrm{C}_k^{\frac{n-1}{2}}(\cos\theta) = \frac{1}{\omega_n} \sum_{l=0}^\infty \frac{b_{2l}^n}{(2l)!} \theta^{2l}. \tag{3.5}$$

Then the Maclaurin spectral coefficients $b_{2l}^n = b_l^n[\Phi]$ can be described by (3.2) *or equivalently by the trace formulation* (3.3)-(3.4).

Now that we have bridged between the Maclaurin spectral coefficients $b_{2l}^n[\Phi]$ of the Schwartzian kernel K_Φ on the one hand and an integral involving the heat trace $\operatorname{tr} e^{s\Delta}$ [*cf.* (3.2)-(3.3)] on the other we go on to exploit this further by showing that the coefficients $b^n_{2l}[\Phi]$ can be described in terms of the classical Jacobi theta functions ϑ_1, ϑ_2. For the sake of the readers convenience we recall that these are defined for $s>0$ respectively by the theta series (*cf.*, e.g., **[9, 25]**)

$$\vartheta_1(s) = 1 + \sum_{j=1}^{\infty} 2e^{-j^2 s} = \sqrt{\pi/s}(1 + \sum_{j=1}^{\infty} 2e^{-j^2\pi^2/s}) \tag{3.6}$$

(where the second equality results from an application of the Poisson summation formula) with asymptotics $\vartheta_1(s) = \sqrt{\pi/s} + O(e^{-1/s})$ as $s \searrow 0$ and

$$\vartheta_2(s) = \sum_{j=0}^{\infty} (2j+1) e^{-\left(j+\frac{1}{2}\right)^2 s}. \tag{3.7}$$

with asymptotics $\vartheta_2(s) \sim 1/s + \sum_{k=0}^{\infty} \mathsf{B}_k s^k/k!$ as $s \searrow 0$ with B_k as in (4.12). We will see below that in odd dimensions it is the function ϑ_1 that will naturally arise and in even dimensions the function ϑ_2.

Theorem 3.2. ($n \geq 3$ *odd*) *Let* $\Phi = \Phi(X)$ *be as in* (3.1). *Then for* $n \geq 3$ *odd the Maclaurin spectral coefficients* $b^n_{2l} = b^n_{2l}[\Phi]$ *in* (3.2)-(3.3) *can be expressed by*

$$b^n_0 = \operatorname{tr} K_\Phi = \sum_{m=0}^{\frac{n-3}{2}} \frac{\mathsf{A}^n_m (-1)^{m+1}}{(n-1)!} \int_0^\infty f(s) \vartheta_1^{(m+1)}(s)\, d\mu, \tag{3.8}$$

where $d\mu(s) = e^{s(n-1)^2/4}\, ds$ *and for* $l \geq 1$ *by*

$$b^n_{2l} = \int_0^\infty f(s) \left[\mathscr{P}^\nu_l \left(-\frac{d}{ds}\right)\right] \operatorname{tr} e^{s\Delta}\, ds = \sum_{m=0}^{\frac{n-3}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}^n_m \mathsf{c}^l_j (-1)^{j+m+1}}{(n-1)!} \times$$
$$\times \binom{j}{i} [(n-1)/2)]^{2i} \int_0^\infty f(s) \vartheta_1^{(m+j-i+1)}(s)\, d\mu.$$

Here c^l_j *are as in Theorem 2.1,* A^n_m *are scalars* (*see below*) *and* $\vartheta_1^{(k)}$ *is the kth derivative of the function* ϑ_1 *as defined by* (3.6).

Proof. We proceed by first writing the heat trace $\Theta(s) = \operatorname{tr} e^{s\Delta}$ in terms of the Jacobi theta function. Towards this end it will be convenient to express the multiplicity function M_n^k in the polynomial form

(3.9)

$$M_k^n = (n+2k-1)\frac{(k+n-2)!}{(n-1)!k!} = \sum_{m=0}^{\frac{n-3}{2}} \frac{2\mathsf{A}_m^n}{(n-1)!}\,(k+(n-1)/2)^{2m+2},$$

where the scalars A_m^n are taken as the coefficients of the polynomial identity $\prod_j (X^2 - j^2) = \sum_m \mathsf{A}_m^n X^{2m+2}$ $(0 \le j, m \le (n-3)/2)$. Using the observation that the sum on the right here vanishes if X is an integer between 1 and $(n-3)/2$ we can write the heat trace as

$$\begin{aligned}\Theta(s) = \operatorname{tr} e^{s\Delta} &= \sum_{k=0}^{\infty} M_k^n e^{-k(k+n-1)s}\\ &= \sum_{m=0}^{\frac{n-3}{2}} \frac{2\mathsf{A}_m^n}{(n-1)!} \sum_{p=1}^{\infty} p^{2m+2} e^{-s\left(p^2-(n-1)^2/4\right)}\\ &= \sum_{m=0}^{\frac{n-3}{2}} \frac{(-1)^{m+1}\mathsf{A}_m^n}{(n-1)!}\vartheta_1^{(m+1)}(s) e^{s(n-1)^2/4}. \qquad (3.10)\end{aligned}$$

One can complete the proof of (3.8) and (3.9) by differentiating (3.10) using Leibniz rule and plugging this into (3.2). □

Theorem 3.3. ($n \ge 2$ *even*) *Let* $\Phi = \Phi(X)$ *be as in* (3.1). *Then for* $n \ge 2$ *even the Maclaurin spectral coefficients* $b_{2l}^n = b_{2l}^n[\Phi]$ *in* (3.2)-(3.3) *can be expressed by*

$$b_0^n = \operatorname{tr} K_\Phi = \sum_{m=0}^{\frac{n-2}{2}} \frac{\mathsf{B}_m^n(-1)^m}{(n-1)!}\int_0^\infty f(s)\vartheta_2^{(m)}(s)\,d\mu, \qquad (3.11)$$

where $d\mu(s) = e^{s(n-1)^2/4}\,ds$ *and for* $l \ge 1$ *by*

(3.12)

$$\begin{aligned}b_{2l}^n &= \int_0^\infty f(s)\left[\mathscr{P}_l^\nu\left(-\frac{d}{ds}\right)\right]\operatorname{tr} e^{s\Delta}\,ds\\ &= \sum_{m=0}^{\frac{n-2}{2}}\sum_{j=1}^{l}\sum_{i=0}^{j} \frac{\mathsf{B}_m^n \mathsf{c}_j^l(-1)^{j+m}}{(n-1)!}\binom{j}{i}[(n-1)/2]^{2i}\int_0^\infty f(s)\vartheta_2^{(m+j-i)}(s)\,d\mu.\end{aligned}$$

Here c_j^l *are as in Theorem 2.1,* B_m^n *are scalars (see below) and* $\vartheta_2^{(k)}$ *is the kth derivative of the function* ϑ_2 *as defined by* (3.7)*.*

Proof. The proof of (3.11) and (3.12) when n is even is very similar to those in the previous theorem and so below we focus on the main differences only. Indeed here we proceed by writing the multiplicity function M_n^k as a polynomial

$$\begin{aligned} M_k^n &= \frac{2k+n-1}{(n-1)!}\prod_{j=1}^{n-2}(k+j) \\ &= \frac{(2k+n-1)}{(n-1)!}\sum_{m=0}^{\frac{n-2}{2}} \mathsf{B}_m^n\left(k+(n-1)/2\right)^{2m}, \end{aligned} \tag{3.13}$$

where the scalars B_m^n are taken as the coefficients of the polynomial identity $\prod_j [X^2-(j-1/2)^2] = \sum_m \mathsf{B}_m^n X^{2m}$ (with $1 \le j \le (n-2)/2$, $0 \le m \le (n-2)/2$) when $n \ge 4$ whilst for $n=2$ the identity on the second line holds trivially with $\mathsf{B}_0^2 = 1$. Using the observation that the sum on the right here vanishes if X is an integer between 1 and $(n-2)/2$ we can write the heat trace as

$$\begin{aligned} \Theta(s) = \mathrm{tr}\, e^{s\Delta} &= \sum_{k=0}^{\infty} M_k^n e^{-k(k+n-1)s} \\ &= \sum_{m=0}^{\frac{n-2}{2}} \frac{2\mathsf{B}_m^n}{(n-1)!}\sum_{p=1/2}^{\infty} p^{2m+1} e^{-s\left(p^2-(n-1)^2/4\right)} \\ &= \sum_{m=0}^{\frac{n-2}{2}} \frac{(-1)^m\mathsf{B}_m^n}{(n-1)!}\vartheta_2^{(m)}(s) e^{s(n-1)^2/4}. \end{aligned} \tag{3.14}$$

The remainder of the argument is similar to that given in Theorem 3.2 and hence abbreviated. $\square$

For the sake of future reference note that in case of the heat kernel [with $\Phi_s(X) = e^{-sX}$] proceeding directly from (3.10)-(3.14) and using the relation $b_{2l}^n[\Phi_s] = b_{2l}^n(s) = \mathscr{P}_l^\nu(-d/ds)\mathrm{tr}\, e^{s\Delta}$ we have for $l \ge 1$:

- For $n \geq 3$ odd b^n_{2l} is given by

(3.15)
$$\sum_{m=0}^{\frac{n-3}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}^n_m \mathsf{c}^l_j (-1)^{m+j+1}}{(n-1)!} \binom{j}{i} \left[(n-1)/2\right]^{2i} \vartheta_1^{(m+j-i+1)} e^{s(n-1)^2/4}.$$

- For $n \geq 2$ even b^n_{2l} is given by

(3.16)
$$\sum_{m=0}^{\frac{n-2}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{B}^n_m \mathsf{c}^l_j (-1)^{m+j}}{(n-1)!} \binom{j}{i} \left[(n-1)/2\right]^{2i} \vartheta_2^{(m+j-i)} e^{s(n-1)^2/4}.$$

Naturally here we have $b^n_0(s) = \Theta(s) = \operatorname{tr} e^{s\Delta}$ as in (3.10) and (3.14) respectively.

4. Asymptotic analysis of Schwartzian kernels via Jacobi functions. Following on from the discussion and representation results in the previous section here we consider a one-parameter family of functions $\Phi_\sigma = \Phi_\sigma(X)$ (with $\sigma > 0$, $X \geq 0$) defined through a Laplace type integral

$$\Phi_\sigma(X) = \int_0^\infty e^{-Xs} f_\sigma(s)\, ds, \qquad X \geq 0, \tag{4.1}$$

where $f_\sigma = f e^{-\sigma s}$ while $|f| \leq c(1 + s^a)$ for some $c > 0$, $a \geq 1$ and all $s > 0$. We aim to describe the asymptotics of $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ as $\sigma \nearrow \infty$ by connecting firstly to the short time behaviour of the heat trace $\Theta(t) = \operatorname{tr} e^{t\Delta}$ and invoking the Minakshisundaram-Pleijel heat coefficients and secondly to the previously encountered Jacobi theta series and their short time asymptotics respectively.

Theorem 4.1. *The Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ with Φ_σ as in* (4.1) *satisfy the asymptotics as $\sigma \nearrow \infty$*

$$b^n_0(\sigma) = \operatorname{tr} \Phi_\sigma(-\Delta) \sim \sum_{k=0}^\infty \frac{a^n_k}{(4\pi)^{n/2}} \int_0^\infty f(s) s^{k-n/2} e^{-\sigma s}\, ds, \tag{4.2}$$

and for $l \geq 1$ *with* $\nu = (n-1)/2$,

$$
\begin{aligned}
b^n_{2l}(\sigma) = \mathrm{tr}\,[\Phi_\sigma \mathscr{P}^\nu_l](-\Delta) \sim \sum_{j=1}^{l} \sum_{k=0}^{\infty} & \frac{(-1)^j \mathsf{c}^l_j(\nu)\Gamma(k-n/2+1)a^n_k}{(4\pi)^{n/2}\Gamma(k-n/2-j+1)} \times \\
& \times \int_0^\infty f(s) s^{k-j-n/2} e^{-\sigma s}\, ds. \qquad (4.3)
\end{aligned}
$$

Proof. Starting from the short time asymptotics of the heat trace (1.3) (*see* **[23]**) for $s > 0$ we have

$$
\begin{aligned}
\Theta(s) = \mathrm{tr}\, e^{s\Delta} &= \sum_{k=0}^{\infty} (2k+n-1)\frac{(k+n-2)!}{k!(n-1)!} e^{-sk(k+n-1)} \\
&= \sum_{k=0}^{\infty} \frac{a^n_k s^k}{(4\pi s)^{n/2}} + O(e^{-1/s}). \qquad (4.4)
\end{aligned}
$$

Therefore successive differentiation with respect to the s-variable results in the expression

$$
\left(-\frac{d}{ds}\right)^j \mathrm{tr}\, e^{s\Delta} = \sum_{k=0}^{\infty} \frac{(-1)^j \Gamma(k-n/2+1)a^n_k}{(4\pi)^{n/2}\Gamma(k-n/2-j+1)} s^{k-j-n/2} + O(e^{-1/s}).
$$

Now referring to the trace formulation of the Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ as in (3.2) we obtain, upon using this last heat trace derivative identity, the description and asymptotics as $\sigma \nearrow \infty$

$$
\begin{aligned}
b^n_{2l}(\sigma) &= \int_0^\infty f_\sigma(s) \left[\mathscr{P}^\nu_l\left(-\frac{d}{ds}\right)\right] \mathrm{tr}\, e^{s\Delta}\, ds \\
&= \int_0^\infty f_\sigma(s) \sum_{j=1}^{l} \mathsf{c}^l_j(\nu) \left(-\frac{d}{ds}\right)^j \mathrm{tr}\, e^{s\Delta}\, ds \\
&\sim \sum_{j=1}^{l} \frac{(-1)^j \mathsf{c}^l_j(\nu)}{(4\pi)^{n/2}} \sum_{k=0}^{\infty} \frac{\Gamma(k-n/2+1)a^n_k}{\Gamma(k-j-n/2+1)} \times \\
&\qquad \times \int_0^\infty f(s) s^{k-j-n/2} e^{-\sigma s}\, ds. \qquad (4.5)
\end{aligned}
$$

Indeed to justify the last line we proceed as follows. First by using the bound on the derivatives of the heat trace $|d^j\Theta(s)/ds^j| \leq cs^{-j-n/2}$

(*see* Appendix C for a proof of this bound) we write for fixed $t > 0$,

$$\left| \left\{ \int_0^\infty - \int_0^t \right\} f_\sigma(s) \frac{d^j}{ds^j} \operatorname{tr} e^{s\Delta} \, ds \right| \le \int_t^\infty |f(s)| s^{-j-n/2} e^{-\sigma s} \, ds.$$

Next, bounding the integral on the right using the bound on f, we can write

$$\begin{aligned} \int_t^\infty |f(s)| s^{-j-n/2} e^{-\sigma s} \, ds &\le c e^{-bt} \int_t^\infty s^{a-j-n/2} e^{-s(\sigma-b)} \, ds \\ &\le \frac{c e^{-bt}}{(\sigma-b)^{a-j-n/2+1}} \int_{(\sigma-b)t}^\infty u^{a-j-n/2} e^{-u} \, du \end{aligned} \tag{4.6}$$

where upon taking $b = \sqrt{|\sigma|}, t = 1$ it is seen that this is of order $O(e^{-\sqrt{|\sigma|}})$. Substituting for $e^{s\Delta}$ and its derivatives in $(0, t)$ using (1.3) and then bounding the remaining integral in an analogous way gives the desired conclusion. □

Theorem 4.2. *Let $n \ge 3$ be odd and let Φ_σ be defined by (4.1) with f_σ as above. Then the Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ satisfy as $\sigma \nearrow \infty$*

$$b^n_0(\sigma) = \operatorname{tr} \Phi_\sigma(-\Delta) \sim \sum_{m=0}^{\frac{n-3}{2}} \frac{\mathsf{A}^n_m \Gamma(m+3/2)}{(n-1)!} \int_0^\infty f(s) s^{-m-3/2} e^{-\sigma s} \, d\mu, \tag{4.7}$$

where $d\mu(s) = e^{s(n-1)^2/4} \, ds$ and for $l \ge 1$

$$\begin{aligned} b^n_{2l}(\sigma) = \operatorname{tr} [\Phi_\sigma \mathscr{P}^\nu_l](-\Delta) &\sim \sum_{m=0}^{\frac{n-3}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}^n_m \mathsf{c}^l_j (-1)^i}{(n-1)!} \binom{j}{i} [(n-1)/2]^{2i} \times \\ &\times \Gamma(m+j-i+3/2) \int_0^\infty f(s) s^{-m-j+i-3/2} e^{-\sigma s} \, d\mu, \end{aligned} \tag{4.8}$$

where A^n_m are the scalars as defined Theorem 3.2.

Proof. Referring to (3.6) we have the asymptotics $\vartheta_1(s) = \sqrt{\pi/s} + O(e^{-1/s})$ as $s \searrow 0$. As a result by successive differentiation for $m \ge 0$

we have for $s \searrow 0$,

$$\begin{aligned} \vartheta_1^{(m+1)}(s) &= (-1)^{m+1} \frac{(2m+1)!!}{2^{m+1}} \sqrt{\pi} s^{-m-3/2} + O(e^{-1/s}) \\ &= (-1)^{m+1} \Gamma\left(m+3/2\right) s^{-m-3/2} + O(e^{-1/s}). \end{aligned} \tag{4.9}$$

Upon substituting these into (3.9) and using the assumptions on f_σ the required asymptotics follows by invoking the same argument as in Theorem 4.1. $\square$

Theorem 4.3. *Let $n \geq 2$ be even and let Φ_σ be defined by (4.1) with f_σ as above. Then the Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ satisfy as $\sigma \nearrow \infty$*

$$\begin{aligned} b^n_0(\sigma) = \operatorname{tr} \Phi_\sigma(-\Delta) \sim & \sum_{m=0}^{\frac{n-2}{2}} \frac{\mathsf{B}^n_m}{(n-1)!} \times \\ & \times \int_0^\infty f(s) \left[\frac{m!}{s^{1+m}} + \sum_{k=m}^\infty \frac{(-1)^m \mathsf{B}_k s^{k-m}}{\Gamma(k-m+1)} \right] e^{-\sigma s} \, d\mu, \end{aligned} \tag{4.10}$$

where $d\mu(s) = e^{s(n-1)^2/4} \, ds$ and for $l \geq 1$

(4.11)

$$\begin{aligned} b^n_{2l}(\sigma) = & \operatorname{tr} [\Phi_\sigma \mathscr{P}^\nu_l](-\Delta) \sim \sum_{m=0}^{\frac{n-2}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{B}^n_m \mathsf{c}^l_j (-1)^{j+m}}{(n-1)!} \binom{j}{i} \left[(n-1)/2\right]^{2i} \times \\ & \times \left\{ \int_0^\infty f(s) \frac{(-1)^{(m+j-i)}(m+j-i)!}{s^{m+j-i+1} e^{\sigma s}} \, d\mu + \right. \\ & \left. + \int_0^\infty f(s) \sum_{k=(m+j-i)}^\infty \frac{\mathsf{B}_k s^{k-m-j+i} e^{-\sigma s}}{\Gamma(k-m-j+i+1)} \, d\mu \right\}, \end{aligned}$$

where B_k are the Bernoulli numbers as defined by (4.12) and B^n_m are the scalars defined in Theorem 3.3.

Proof. It is enough here to use the fact that the theta series defining ϑ_2 satisfies the asymptotics as $s \searrow 0$

$$\vartheta_2(s) \sim \frac{1}{s} + \sum_{k=0}^\infty \frac{\mathsf{B}_k s^k}{k!}, \qquad \mathsf{B}_k = \frac{(-1)^k}{(k+1)} B_{2k+2} \left(1 - 2^{-2k-1}\right) \tag{4.12}$$

where B_m are the well-known Bernoulli numbers and likewise by further differentiating that

$$\vartheta_2^{(m)}(s) \sim \frac{(-1)^m m!}{s^{1+m}} + \sum_{k=m}^{\infty} \frac{\mathsf{B}_k s^{k-m}}{\Gamma(k-m+1)} \tag{4.13}$$

as $s \searrow 0$ (*cf.* **[9, 25]**). Substituting these into (3.12) and using the assumptions on f_σ leads to (4.11). $\square$

Trace asymptotics and resolvent powers. As an application we here discuss the asymptotics of the powers of the resolvent corresponding to taking $f_\sigma(s) = s^{a-1}e^{-s\sigma}/\Gamma(a)$ for $a > 1$. Through a limiting process these will then be used to obtain the asymptotics for the Maclaurin spectral coefficients of the heat kernel, that is, $b_{2l}^n[\Phi = e^{-tX}]$. Indeed let

$$\Phi_\sigma(X) = \int_0^\infty \frac{s^{a-1}e^{-s\sigma}}{\Gamma(a)} e^{-sX}\, ds = (\sigma + X)^{-a}. \tag{4.14}$$

Then $\Phi_\sigma(-\Delta) := R_\sigma^a$ is the resolvent operator to the power a. By applying the theorems of Section 4 we can obtain the asymptotics of the Maclaurin spectral coefficients $b_{2l}^n(\sigma, a) = b_{2l}^n[R_\sigma^a]$ as $\sigma \nearrow \infty$. To this end note that Theorem 4.1 gives (for $l \geq 1$)

(4.15)

$$b_{2l}^n(\sigma, a) \sim \sum_{j=0}^{l} \sum_{k=0}^{\infty} \frac{(-1)^j \mathsf{c}_j^l(\nu)\Gamma(k-n/2+1)\Gamma\left(a+k-j-n/2\right)}{(4\pi)^{n/2}\Gamma(k-n/2-j+1)\Gamma(a)\sigma^{a+k-j-n/2}} a_k^n.$$

Alternatively by invoking the theta function description of the Maclaurin spectral coefficients we have the following asymptotics by considering the cases of odd and even n separately.

- For $n \geq 3$ odd Theorem 4.2 yields

(4.16)

$$b_0^n(\sigma, a) \sim \sum_{m=0}^{\frac{n-3}{2}} \frac{\mathsf{A}_m^n \Gamma(m+3/2)}{(n-1)!\Gamma(a)} \Gamma\left(a-m-3/2\right)\left(\sigma-(n-1)^2/4\right)^{m-a+3/2},$$

and for $l \geq 1$,

(4.17)

$$b_{2l}^n(\sigma, a) \sim \sum_{m=0}^{\frac{n-3}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}_m^n \mathsf{c}_j^l (-1)^i}{(n-1)!\Gamma(a)} \binom{j}{i} [(n-1)/2]^{2i} \, \Gamma(m+j-i+3/2)$$
$$\times \Gamma(a+i-m-j-3/2) \left(\sigma - (n-1)^2/4\right)^{m+j-i-a+3/2}.$$

- For $n \geq 2$ even Theorem 4.3 yields

(4.18)

$$b_0^n(\sigma, a) \sim \sum_{m=0}^{\frac{n-2}{2}} \frac{\mathsf{B}_m^n}{(n-1)!\Gamma(a)} \Bigg\{ m!\Gamma(a-1-m) \left(\sigma - (n-1)^2/4\right)^{1-a+m} +$$
$$+ \sum_{k=m}^{\infty} (-1)^m \frac{\mathsf{B}_k \Gamma(a+k-m)}{\Gamma(k-m+1)} \left(\sigma - (n-1)^2/4\right)^{-a-k+m} \Bigg\},$$

and for $l \geq 1$,

(4.19)

$$b_{2l}^n(\sigma, a) \sim \sum_{m=0}^{\frac{n-2}{2}} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{B}_m^n \mathsf{c}_j^l (-1)^{j+m}}{(n-1)!\Gamma(a)} \binom{j}{i} [(n-1)/2]^{2i} \Bigg\{ (-1)^{(m+j-i)}$$
$$\times (m+j-i)!\Gamma(a-1-m-j+i) \left(\sigma - (n-1)^2/4\right)^{1-a+m+j-i} +$$
$$+ \sum_{k=(m+j-i)}^{\infty} \frac{\mathsf{B}_k \Gamma(a+k-m-j+i)}{\Gamma(k-m-j+i+1)} \left(\sigma - (n-1)^2/4\right)^{-a-k+m+j-i} \Bigg\}.$$

The asymptotics of $b_0^n(\sigma, a)$ as $\sigma \nearrow \infty$ now give the short time asymptotics of the heat trace. This follows by first noting $\Theta(s) = \operatorname{tr} e^{s\Delta} = \lim (k/s)^k \operatorname{tr} R_{k/s}^k = \lim (k/s)^k b_0^n(k/s, k)$ as $k \nearrow \infty$ for $s > 0$ and recalling $e^{-x} = \lim(1+x/k)^{-k}$ and $\lim \Gamma(k+\alpha)/[\Gamma(k)k^\alpha] = 1$ as $k \nearrow \infty$ for $\alpha \in \mathbb{R}$. Now for $n \geq 3$ odd using (4.16) this leads to (as $s \searrow 0$)

$$\operatorname{tr} e^{s\Delta} \sim e^{s(n-1)^2/4} \sum_{m=0}^{\frac{n-3}{2}} \frac{\mathsf{A}_m^n \Gamma(m+3/2)}{(n-1)!} s^{-m-3/2}, \tag{4.20}$$

and in a similar fashion for $n \geq 2$ even using (4.19) this leads to (as $s \searrow 0$)

$$\operatorname{tr} e^{s\Delta} \sim e^{s(n-1)^2/4} \sum_{m=0}^{\frac{n-2}{2}} \frac{\mathsf{B}_m^n (-1)^m}{(n-1)!} \times \times \left\{ (-1)^m (m!) s^{-m-1} + \sum_{k=m}^{\infty} \frac{\mathsf{B}_k s^{k-m}}{\Gamma(k-m+1)} \right\}. \tag{4.21}$$

Compare with (3.10)-(3.14) and (3.15)-(3.16).

5. Dirichlet energy and extension by semigroups. In this section we apply some of the tools developed earlier to build and study extension operators out of semigroups $(T_t : t > 0)$ generated by functions of the spherical Laplacian and some energy inequalities resulting from them. Here the extension operator extends functions on the n-sphere $\mathbb{S}$ – seen as the boundary of the open unit ball $\mathbb{B} = \{(x_1, ..., x_{n+1}) : |x| \leq 1\}$ – to functions inside the ball by a fixed semigroup and the aim is to examine the associated energy inequalities by invoking the Maclaurin spectral coefficients and the classical Funk-Hecke identity. For the sake of this exposition we confine to the Dirichlet energy and Dirichlet principle asserting that for all $f \in H^{1/2}(\mathbb{S}) \subset L^2(\mathbb{S})$ and with u_H denoting the harmonic extension of f to $\mathbb{B}$ we have

$$\int_{\mathbb{B}} |\nabla u|^2 \geq \int_{\mathbb{B}} |\nabla u_H|^2, \qquad \forall u \in H^1(\mathbb{B}) : u|_{\partial \mathbb{B}} = f. \tag{5.1}$$

To this end, let $F = F(X)$ be a non-negative function in the Borel functional calculus of the spherical Laplacian Δ and for $0 < r \leq 1$ consider the associated one parameter family of functions $\Phi_r = \Phi_r(X)$ defined as

$$\Phi_r(X) = r^{F(X)}. \tag{5.2}$$

The operator family $(\Phi_r(-\Delta) : 0 < r \leq 1)$ is then a semigroup in $L^2(\mathbb{S})$; in fact, the substitution $r = e^{-t}$ shows that $\Phi_r(-\Delta)$ is a re-parametrisation of the semigroup $(T_t = e^{-tF(-\Delta)} : t \geq 0)$. Now writing the expansion of f in spherical harmonics $f = \sum_{k=0}^{\infty} Y_k$ where Y_k are spherical harmonics of degree k, we define the extension u_F of f to be

$$
\begin{aligned}
u_F(rx) = \Phi_r(-\Delta)f(x) &= \sum_{k=0}^{\infty} r^{F(\lambda_k^n)} Y_k(x) \qquad x \in \mathbb{S}, \quad 0 < r \le 1, \\
&= \int_{\mathbb{S}} K_{\Phi_r}(x,y) f(y)\, d\mathcal{H}^n(y), \qquad (5.3)
\end{aligned}
$$

where K_{Φ_r} is the Schwartzian kernel of $\Phi_r(-\Delta)$ [*cf.* (5.9) for a formulation]. Note that upon taking $F = H$ with H the function

$$
H(X) := \left(X + \left(\frac{n-1}{2} \right)^2 \right)^{1/2} - \frac{n-1}{2}, \qquad X \ge 0, \tag{5.4}
$$

we have $H(\lambda_k^n) = k$ for all $k \ge 0$ and subsequently u_H is precisely the harmonic extension of f to the unit ball. Now using the identity

$$
\int_{\mathbb{B}} |\nabla u_F|^2 = \int_0^1 \int_{\mathbb{S}} \left[|\partial_r u_F|^2 - \frac{1}{r^2} u_F \Delta_{\mathbb{S}} u_F \right] r^n \, d\mathcal{H}^n dr, \tag{5.5}
$$

it can be seen that the Dirichlet energy of u_F as defined by (5.3) can be expressed as

$$
\int_{\mathbb{B}} |\nabla u_F|^2 = \sum_{k=0}^{\infty} \left[\frac{F(\lambda_k^n)^2 + \lambda_k^n}{2F(\lambda_k^n) + n - 1} \right] \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n. \tag{5.6}
$$

In particular the energy of the harmonic extension u_H can ben seen to be

$$
\begin{aligned}
\int_{\mathbb{B}} |\nabla u_H|^2 &= \sum_{k=0}^{\infty} \left[\frac{H(\lambda_k^n)^2 + \lambda_k^n}{2H(\lambda_k^n) + n - 1} \right] \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n \\
&= \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n = ||f||^2_{H^{1/2}(\mathbb{S})}. \qquad (5.7)
\end{aligned}
$$

Thus in view of $u_F = u_H = f$ on $\partial\mathbb{B}$ the Dirichlet principle is a formulation of the inequality

$$
\sum_{k=0}^{\infty} \left[\frac{F(\lambda_k^n)^2 + \lambda_k^n}{2F(\lambda_k^n) + n - 1} \right] \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n \ge \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n. \tag{5.8}
$$

We now use the Funk-Hecke formula to give an alternative expression of the Dirichlet energy of u_F using the Maclaurin spectral coefficients.

The Schwartzian kernel of Φ_r can be written via Gegenbauer polynomials as

$$
\begin{aligned}
K_{\Phi_r}(x,y) &= \frac{1}{\omega_n}\sum_{k=0}^{\infty} M_k^n \Phi_r(\lambda_k^n) \mathrm{C}_k^{\frac{n-1}{2}}(\cos\theta) \\
&= \frac{1}{\omega_n}\sum_{k=0}^{\infty}(2k+n-1)\frac{(k+n-2)!}{k!(n-1)!} r^{F(\lambda_k^n)} \mathrm{C}_k^{\frac{n-1}{2}}(\cos\theta) \qquad (5.9)
\end{aligned}
$$

where $\theta = \cos^{-1}(x \cdot y)$ is the geodesic distance from x to y. By formally writing the Maclaurin expansion of the kernel K_{Φ_r} we have

$$
\sum_{k=0}^{\infty}(2k+n-1)\frac{(k+n-2)!}{k!(n-1)!} r^{F(\lambda_k^n)} \mathrm{C}_k^{\frac{n-1}{2}}(\cos\theta) = \sum_{l=0}^{\infty} \frac{b_{2l}^n(r)}{(2l)!}\theta^{2l} \qquad (5.10)
$$

where the Maclaurin spectral coefficients $b_{2l}^n(r) = b_{2l}^n[\Phi_r]$, by referring to the earlier description, can be written as

$$
b_{2l}^n(r) = \sum_{k=0}^{\infty} M_k^n \Phi_r(\lambda_k^n) \sum_{j=1}^{l} c_j^l [\lambda_k^n]^j = \sum_{k=0}^{\infty} M_k^n [\Phi_r \mathscr{P}_l](\lambda_k^n). \qquad (5.11)
$$

Using the Funk-Hecke formula on the integral operator below (*cf.* **[18, 21]** or **[17]**) we therefore have

$$
\begin{aligned}
u_F(rx) &= \int_{\mathbb{S}^n} K_{\Phi_r}(x,y) f(y)\, d\mathcal{H}^n(y) \qquad x \in \mathbb{S}, \quad 0 < r \le 1, \\
&= \sum_{l=0}^{\infty}\sum_{k=0}^{\infty} \frac{b_{2l}^n(r)}{\omega_n (2l)!} \int_{\mathbb{S}^n} \left[\cos^{-1}(x\cdot y)\right]^{2l} Y_k(y)\, d\mathcal{H}^n(y) \\
&= \sum_{l=0}^{\infty}\sum_{k=0}^{\infty} \frac{\mu_k^l b_{2l}^n(r)}{\omega_n (2l)!} Y_k(x) \qquad (5.12)
\end{aligned}
$$

where the coefficients μ_k^l are explicitly given by the weighted integral

$$
\mu_k^l = \omega_{n-1} \int_{-1}^{1} \left[\cos^{-1}(t)\right]^{2l} \mathrm{C}_k^{(n-1)/2}(t)(1-t^2)^{\frac{n-1}{2}}\, dt, \quad l \ge 0. \qquad (5.13)
$$

Invoking (5.1) and (5.5) and directly comparing the expansions in spherical harmonics of the extension u_F given by (5.3) with (5.12) leads at once to the following statement.

Theorem 5.1. *Given $F = F(X)$ as above and $f \in H^{1/2}(\mathbb{S})$ let $u_F = r^{F(-\Delta)} f$ denote the extension of f as defined by* (5.3). *Then the Dirichlet energy of u_F can be written as the weighted sum:*

$$\int_{\mathbb{B}} |\nabla u_F|^2 = \sum_{k=0}^{\infty} \int_0^1 \left[\gamma_k'^2(r) + \frac{1}{r^2} \gamma_k^2(r) \lambda_k^n \right] r^n \, dr \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n, \tag{5.14}$$

where the functions $\gamma_k = \gamma_k(r)$ and the Maclaurin spectral coefficients $b_{2l}^n(r) = b_{2l}^n[r^{F(-\Delta)}]$ satisfy the trace formulation

$$\gamma_k(r) = \sum_{l=0}^{\infty} \frac{b_{2l}^n(r)}{(2l)!} \mu_k^l = \mathrm{tr} \left[\sum_{l=0}^{\infty} \frac{\mu_k^l}{(2l!)} r^{F(-\Delta)} P_l(-\Delta) \right] = r^{F(\lambda_k^n)}, \tag{5.15}$$

with the sequence μ_k^l given by (5.13). *Furthermore we have the energy inequality*

$$\sum_{k=0}^{\infty} \int_0^1 \left[\gamma_k'^2(r) + \frac{1}{r^2} \gamma_k^2(r) \lambda_k^n \right] r^n \, dr \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n \geq \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n. \tag{5.16}$$

In particular in view of the arbitrariness of the boundary function $f \in L^2(\mathbb{S})$ or else a direct variational argument the above energy inequality results in the following.

Corollary 5.1. *Let $\gamma_k = \gamma_k(r)$ be as given by the trace formulation* (5.15) *and set $h_k(r) = r^k$. Then for all $k \geq 0$ we have $\mathbb{E}_k[\gamma_k] \geq \mathbb{E}_k[h_k]$, that is,*

$$\int_0^1 \left[\gamma_k'^2(r) + \frac{\lambda_k^n}{r^2} \gamma_k^2(r) \right] r^n \, dr \geq \int_0^1 \left[h_k'^2(r) + \frac{\lambda_k^n}{r^2} h_k^2(r) \right] r^n \, dr. \tag{5.17}$$

Here $\lambda_k^n = k(n+k-1)$ are the distinct eigenvalues of the spherical Laplacian while by direct verification $\mathbb{E}_k[h_k] = k$.

Proof. Fix $k \geq 0$ and let g in $H^1(0,1)$ satisfy $g(0) = 0$, $g(1) = 1$. Then firstly for $h = h_k$ as above it is seen that $-d/dr[r^n h_k'(r)] + \lambda_k^n r^{n-2} h_k(r) = 0$. Secondly upon writing $g = h + \phi$ with $\phi \in H_0^1(0,1)$ and invoking the quadratic nature of the energy we can write $\mathbb{E}_k[g] = \mathbb{E}_k[h + \phi] = \mathbb{E}_k[h] + \mathbb{E}_k[\phi] \geq \mathbb{E}_k[h] = k$ with the last inequality being *strict* for non-zero ϕ. Thus $h = h_k$ is the unique minimiser of $\mathbb{E}_k$ with respect to its own boundary conditions. $\square$

Now to finish-off the section we give a few examples to illustrate the above discussion of energy inequalities.

- If $F(X) \equiv s$ for some fixed $s \in [0, \infty)$ then u_F is the homogeneous degree s extension of f, that is, $u_F(rx) = r^s f(x)$. Moreover

$$\begin{aligned}\int_{\mathbb{B}} |\nabla u_F|^2 &= \sum_{k=0}^{\infty} \frac{s^2 + \lambda_k^n}{2s + n - 1} \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n \\ &= \frac{s^2 \|f\|^2_{L^2(\mathbb{S})} + \|\nabla f\|^2_{L^2(\mathbb{S})}}{2s + n - 1} \geq \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n.\end{aligned}$$

Interestingly taking the infimum on the left over $s \geq 0$ and rearranging terms leads to the inequality

$$\sqrt{(n-1)^2 ||f||^4_{L^2(\mathbb{S})} + 4 ||\nabla f||^2_{L^2(\mathbb{S})} ||f||^2_{L^2(\mathbb{S})}} \geq \sum_{k=0}^{\infty} (2k + n - 1) \int_{\mathbb{S}} |Y_k|^2.$$

- If $F(X) = X$ then $F(-\Delta)$ is the spherical Laplacian and $u_F = e^{t\Delta} f$ with $t = \log 1/r$ is the heat extension of f. Here $\gamma_k(r) = r^{k(k+n-1)}$ and

$$\int_{\mathbb{B}} |\nabla u_F|^2 = \sum_{k=0}^{\infty} \frac{\lambda_k^n (1 + \lambda_k^n)}{2\lambda_k^n + n - 1} \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n \geq \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n.$$

- Pick $F_s(X)$ such that $F_s(\lambda_k^n) = sk$ for some fixed $s \in [0, \infty)$. (Note that $u_{F_1} = u_H$ is the harmonic extension of f.) Then $\gamma_k(r) = r^{sk}$ and we have

$$\int_{\mathbb{B}} |\nabla u_{F_s}|^2 = \sum_{k=0}^{\infty} \frac{k \left(s^2 k + k + n - 1 \right)}{2\, sk + n - 1} \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n \geq \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 \, d\mathcal{H}^n.$$

We remark that the last inequality is saturated when $s = 1$.

Appendices

In this appendix we gather together some of the results and calculations relating to the Gegenbauer and Bell polynomials that appeared earlier in the paper. [1]

A. Gegenbauer polynomials C_k^ν ($k \geq 0$, $\nu > -1/2$). The Gegenbauer or ultraspherical polynomial $C_k^\nu(t)$ ($k \geq 0, \nu > -1/2$) is defined by the coefficient of α^k in the generating function relation

$$\frac{1}{(1-2t\alpha+\alpha^2)^\nu} = \sum_{k=0}^{\infty} C_k^\nu(t)\alpha^k. \tag{A.1}$$

It has a truncated series representation resulting from the series solution to the Gegenbauer differential equation (*see* below) in the form

$$C_k^\nu(t) = \sum_{0\leq l\leq \frac{k}{2}} (-1)^l \frac{\Gamma(k-l+\nu)}{\Gamma(\nu)l!(k-2l)!}(2t)^{k-2l}, \tag{A.2}$$

and most notably the derivatives satisfy the recursive relation

$$\frac{d^m}{dt^m} C_k^\nu(t) = 2^m \frac{\Gamma(\nu+m)}{\Gamma(\nu)} C_{k-m}^{\nu+m}(t). \tag{A.3}$$

The polynomial $y = C_k^\nu(t)$ is a solution to the second-order homogenous differential equation (the Gegenbauer equation)

$$\left(1-t^2\right)\frac{d^2y}{dt^2} - (2\nu+1)t\frac{dy}{dt} + k(k+2\nu)y = 0, \tag{A.4}$$

that constitute a regular Sturm-Liouville system on the interval $(-1,1)$. The corresponding Gegenbauer operator is seen to be a positive self-adjoint second order differential operator in the weighted Lebesgue-Hilbert space $L^2(-1,1;(1-t^2)^{\nu-1/2}dt)$ having the discrete spectrum $\lambda_k = k(k+2\nu) : k \geq 0$ with associated eigenfunctions $y = C_k^\nu(t)$. In particular upon setting $d\mu = (1-t^2)^{\nu-1/2}dt$ we have the orthogonality

[1] For more on Gegenbauer polynomials and applications *cf.* **[?, 26, 32]**.

relations

$$(C_k^\nu, C_m^\nu)_{L^2(d\mu)} = \int_{-1}^{1} C_k^\nu(t)\, C_m^\nu(t) \left(1-t^2\right)^{\nu-1/2} dt$$

$$= \frac{\pi 2^{1-2\nu}\Gamma(2\nu+m)}{m!(m+\nu)\Gamma(\nu)^2}\delta_{km}, \qquad k,m \geq 0, \tag{A.5}$$

where δ_{km} denotes the Kronecker delta. By direct evaluation using (A.2) or otherwise we have the pointwise identities $C_k^\nu(1) = (2\nu)_k/k!$, $C_k^\nu(-t) = (-1)^k C_k^\nu(t)$ where $(x)_k = \Gamma(x+k)/\Gamma(x)$. When necessary we use the normalised form of the polynomial defined by

$$\mathscr{C}_k^\nu(t) = \frac{C_k^\nu(t)}{C_k^\nu(1)}, \qquad C_k^\nu(1) = \frac{\Gamma(2\nu+k)}{\Gamma(2\nu)k!}. \tag{A.6}$$

B. The Bell polynomials $\mathsf{B}_{m,j}$ and the vanishing of $\mathsf{B}_{2l,j}$ for $l \geq 1$, $j \geq l+1$. To describe the action of the differential operator $\mathscr{L} = \mathsf{P}(d/d\theta)$ associated with the polynomial $\mathsf{P} = \mathsf{P}_d(X)$ of degree $d \geq 2$ on the Gegenbauer polynomials we will make use of Faà di Bruno's formula, a generalised chain rule, in order to write derivatives of $\mathscr{C}_k^\nu$ in term of the (*incomplete*) Bell polynomials. Recall that for a pair of positive integers m, j the Bell polynomial $\mathsf{B}_{m,j}$ is the multi-variable polynomial defined for $x = (x_1, \dots, x_{m-j+1})$ as

$$\mathsf{B}_{m,j}(x) = \sum \frac{m!}{k_1!k_2!\dots k_{m-j+1}!} \prod_{i=1}^{m-j+1} \left(\frac{x_i}{i!}\right)^{k_i} \tag{B.1}$$

where the sum is taken over all sequences of non-negative integers $k_1, \dots, k_{m-j+1}$ such that [2]

$$k_1 + \cdots + j_{m-j+1} = j, \text{ and } k_1 + 2k_2 + \cdots + (m-j+1)k_{m-j-1} = m. \tag{B.2}$$

For smooth functions f, g and $m \geq 1$, Faà di Bruno's formula then asserts that

(B.3)

$$\frac{d^m}{dx^m} f(g(x)) = \sum_{j=1}^{m} f^{(j)}(g(x)) \cdot \mathsf{B}_{m,j}\left(g'(x), g''(x), \dots, g^{(m-j+1)}(x)\right).$$

[2] The coefficients of the Bell polynomials relate to the number of ways a given set can be partitioned and thus have many applications in combinatorics (*cf.* **[6]** for more).

We now make the following useful observation which will simplify certain applications of Faà di Bruno's formula.

Lemma B.1. $\mathsf{B}_{2l,j}(0, x_2, x_3, \ldots, x_{2l-j+1}) \equiv 0$ *for* $l \geq 1$ *when* $j \geq l+1$.

Proof. It suffices to show that here the terms in $\mathsf{B}_{2l,j}$ depend on the first variable. This amounts to showing that if $j \geq l+1$, $(k_i : 1 \leq i \leq 2l-j+1)$ satisfy (B.2) with $m = 2l$ then $k_1 \neq 0$. Indeed let $(k_i : 1 \leq i \leq 2l-j+1)$ be non-negative integers such that (B.2) are satisfied but $k_1 = 0$. Then $\sum k_i = j \geq l+1$ with $2 \leq i \leq 2l-j+1$. On the other hand because of the second condition in (B.2) being true we have

$$\sum_{i=2}^{2l-j+1} ik_i = \sum_{i=2}^{2l-j+1} (i-2)k_i + 2\sum_{i=2}^{2l-j+1} k_i \geq 2(l+1) > 2l, \tag{B.4}$$

which is an evident contradiction. This therefore completes the proof. $\square$

C. Bounds on the derivatives of $\operatorname{tr} e^{t\Delta}$**.** Let M be a complete Riemannian manifold we recall that there exists $c > 0$ such that

$$\left|\operatorname{tr} e^{z\Delta}\right| \leq c\Re(z)^{-n/2} \tag{C.1}$$

for all $\Re(z) > 0$. We also recall that the trace of the heat kernel is analytic in z for $\Re(z) > 0$. Let γ be the circle in $\mathbb{C}$ with center $s \in (0, \infty)$ and radius $s/2$. Then if $z \in \gamma$ we have $s/2 \leq \Re(z) \leq 3s/2$. Therefore, using Cauchy's integral formula, we have

$$\begin{aligned} \left|\frac{d^j}{ds^j} \operatorname{tr} e^{s\Delta}\right| &= \left|\frac{1}{2\pi i}\oint_\gamma \frac{\operatorname{tr} e^{-z\Delta}}{(z-s)^{j+1}}\, dz\right| \\ &\leq \frac{c}{2\pi s^{j+1}}\oint_\gamma \Re(z)^{-n/2}\, dz \leq c\left(\frac{3}{2}\right)^{-n/2} s^{-n/2-j}. \end{aligned} \tag{C.2}$$

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Department of Mathematics, University of Sussex, Brighton, UK
Email address: **s.day@sussex.ac.uk**

Department of Mathematics, University of Sussex, Brighton, UK
Email address: **a.taheri@sussex.ac.uk**